Soil moisture data as a constraint for groundwater recharge estimation

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Abstract

Estimating groundwater recharge rates is important for water resource management studies. Modeling approaches to forecast groundwater recharge typically require observed historic data to assist calibration. It is generally not possible to observe groundwater recharge rates directly. Therefore, in the past, much effort has been invested to record soil moisture content (SMC) data, which can be used in a water balance calculation to estimate groundwater recharge. In this context, SMC data is measured at different depths and then typically integrated with respect to depth to obtain a single set of aggregated SMC values, which are used as an estimate of the total water stored within a given soil profile. This article seeks to investigate the value of such aggregated SMC data for conditioning groundwater recharge models in this respect. A simple modeling approach is adopted, which utilizes an emulation of Richards' equation in conjunction with a soil texture pedotransfer function. The only unknown parameters are soil texture. Monte Carlo simulation is performed for four different SMC monitoring sites. The model is used to estimate both aggregated SMC and groundwater recharge. The impact of conditioning the model to the aggregated SMC data is then explored in terms of its ability to reduce the uncertainty associated with recharge estimation. Whilst uncertainty in soil texture can lead to significant uncertainty in groundwater

recharge estimation, it is found that aggregated SMC is virtually insensitive to soil texture.

Keywords: Conditioning, Groundwater recharge, Soil moisture content, Soil texture, Vertical percolation

1. Introduction

An essential aspect of water resource planning often involves the estimation of groundwater recharge rates, here defined as the rate at which water arrives at the water table of an aquifer following precipitation, interception, snow melt, evapotranspiration and percolation through the unsaturated zone. In many cases, water loss during percolation through the unsaturated zone below the reach of plant roots can be assumed negligible. Consequently, vertical percolation beneath the reach of plant roots and groundwater recharge are often treated as being the same (Quinn et al., 2012; Sorensen et al., 2014). Hereafter, vertical percolation is referred to as a proxy for groundwater recharge. Vertical percolation rates (VPR) can be estimated using a multitude of different models, all of which require historic data of some form to enable appropriate model parameter calibration.

Ideally, such models should be calibrated to observed groundwater recharge rates. However, groundwater recharge data is difficult to observe directly. Some studies have sought to derive recharge data by separating out base flow from river discharge rate records (Rutledge, 2007). The problem here is that base flow separation methods are, in themselves, *ad hoc* and unconstrained, unless combined with some form of tracer based mass balance study (Lott and Stewart, 2016). Another method is to assume a specific yield for an unconfined aquifer and to infer recharge rates

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from water table changes (Healy and Cook, 2002). The problem with this latter approach is that there is often significant uncertainty about the time-varying characteristics of specific yield (Healy and Cook, 2002; Mathias and Butler, 2006) and significant care is required to properly take into account the effects of lateral groundwater flow rates (Healy and Cook, 2002; Cuthbert et al., 2016).

Arguably, the most direct method of observing recharge rates is to measure VPR from an in situ lysimeter (von Freyberg et al., 2015). The issue here is that such facilities are very expensive to manage and very few facilities exist around the world.

Another related approach is to continuously monitor moisture content within a soil profile over a long period of time (Ireson et al., 2006). Providing that precipitation (net of interception) and actual evapotranspiration (AE) are also monitored, soil moisture content (SMC) data can be used to develop a VPR measurement by water balance. However, a problem is that AE is not often measured. Instead, an estimate of potential evapotranspiration (PE) is generally obtained using weather station data (incoming radiation, temperature, humidity, wind speed etc.) in conjunction with an appropriate physics model (e.g. Allen et al., 1998). Under such conditions, a direct estimate of VPR is not possible by water balance, as the quantity of AE is unknown. Consequently, VPR must instead be estimated by simulating soil-plant-water processes using an appropriate model, which is conditioned to the observed SMC data.

Interestingly, previous modeling studies have focused on the ability of models to estimate SMC data as opposed to the value of SMC data as a conditioner for estimating VPR (Ragab et al., 1997; Sorensen et al., 2014). In a recent study, Sorensen et al. (2014) presented SMC content data from four instrumented sites from southern England. They then compared estimated SMC data from four different uncalibrated recharge estimation methods. The authors conclude that, whilst each of four models provided a “generally good agreement” between simulated and observed SMC, there were large discrepancies between the different VPR estimates, leading to concerns over the value of SMC data for conditioning groundwater recharge modeling in the future.

In the current study, the four aforementioned instrumented sites presented by Sorensen et al. (2014) are revisited to quantify the extent to which observed SMC data can be used to reduce uncertainty associated with groundwater recharge in the context of a single model structure. In particular, the model structure used includes a recently developed soil moisture accounting procedure (SMAP) designed by Mathias et al. (2015), which is described later on in this article. Unknown input parameters associated with this SMAP only include information about the soil texture of the site (i.e., % clay, % silt and % sand).

The outline of this article is as follows. An explanation is provided concerning the data, models and conditioning strategies to be applied. The aforementioned SMAP is used to estimate VPR at the four instrumented sites in southern England. Probability of non-exceedance (PNE) confidence limits are acquired using four successive methodologies. For comparison, PNE confidence limits are first acquired assuming any soil texture is equally likely to be applicable at each of the four sites. PNE confidence limits are then refined by conditioning the SMAP to the observed SMC data from each site. For further comparison, an additional set of PNE confidence limits is acquired by restricting soil texture to be within a polygon on a soil texture ternary diagram associated with the soil texture classification for that site as designated by the UK soil observatory (UKSO). The results are compared and contrasted so as to draw wider conclusions with regards to the value of observed SMC data when seeking to estimate VPR for groundwater recharge studies in the future.

2. Data and methodology

2.1. Data

The data used for this study include daily net rainfall (i.e., rainfall minus canopy interception losses) and PE data in conjunction with observed SMC from the four instrumented sites previously discussed by Sorensen et al. (2014). The four sites include Warren Farm, Highfield Farm, Beche Park Wood and Grimsbury Wood, all of which are located in Berkshire, UK.

Daily net rainfall and AE data were obtained by Sorensen et al. (2014) using JULES (Best et al., 2011) driven by nearby meteorological observations. A default JULES parameterisation was used for grassland sites with woodland vegetation parameters defined using observations by Herbst et al. (2008).

Routine SMC data were obtained at each site as follows (Sorensen et al., 2014). Point measurements of SMC were obtained using neutron probes at 17 intervals at depths of 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.8, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.3, 2.6, 2.9, 3.2 m, respectively. The results were then aggregated together, by depth weighting, to obtain a depth of water contained within the top 3 m of the soil profile.

Soil texture maps from the UK soil observatory (UKSO, 2016) were used to provide soil texture data describing the surface cover of the four sites.

The UKSO map covers Great Britain and integrates geology and soil characteristics at a scale of 1:50 000, with a 1 km resolution version available for regional overviews. The simplified soil texture classifications are derived from measured soil textures (% clay, % silt and % sand) taken from archive samples held by the British Geological Survey. The map uses terms that refer to:

sandy soils, silty soils, clayey soils and loamy soils with additional indicators for the presence of chalk fragments (chalky) and peat (peaty). For reference, soil texture ternary diagrams illustrating the various available UKSO soil texture classifications are presented in Fig. 1.

2.2. Geology and soil cover of the field sites

Location maps of the four field sites, Warren Farm, Highfield Farm, Beche Park Wood and Grimsbury Wood, have previously been presented by Sorensen et al. (2014). The four locations cover a range of different superficial geology, soil type and land use. Warren Farm and Highfield Farm are grassland sites. Beche Park Wood and Grimsbury Wood are deciduous woodland sites. All four sites are underlain by chalk geology, with water tables located at greater than 10 m depth. The Chalk in this area is overlain by superficial clay-with-flints formation or Paleogene deposits comprising of clays, interbedded sands and silty clays with the exception of Warren Farm which is chalk outcrop (Sorensen et al., 2014).

Soil logs indicate the following (Sorensen et al., 2014): Warren Farm consists of a thin 0.2 m soil, including flints, overlying weathered chalk which grades into consolidated chalk between 1 and 3 m depth. Highfield Farm consists of a very heterogeneous fine loam to around 0.4 to 0.5 m, above clay with various degrees of interbedded gravel. Beche Park Wood consists of around 0.3 m of gravely clay, over clay-with-flints containing occasional sand filled fissures. Grimsbury Wood is predominantly silty clay overlain by 0.3 m of loam.

The soil texture for the four sites according to UKSO is as follows: Warren Farm is described as a “chalky silty loam”. Highfield Farm is described as “loam to sand”. Beche Park Wood is described as “clay to clayey loam”. Grimsbury Wood is described as “clay to silt”.

The UKSO map provides quite reasonable soil texture descriptions for Beche Park Wood and Grimsbury Wood. However,the UKSO map soil texture descriptions do not compare well with the field descriptions for Warren Farm and Highfield Farm, previously provided by Sorensen et al. (2014). Indeed there are many problems associated with determining soil texture for soils associated with chalk (Kerry et al., 2009). Nevertheless, the UKSO soil textures will be considered further as an alternative conditioner for groundwater recharge estimation.

2.3. Vertical percolation rate (VPR) modeling

The soil moisture accounting procedure (SMAP) previously proposed by Mathias et al. (2015) was used to simulate VPR at the four sites. The model requires daily net rainfall, PE data and soil texture data to provide estimates of aggregated SMC and VPR.

The SMAP has been specifically designed to emulate Richards' equation in conjunction with the plant roots stress function of Feddes et al. (1976) and the pedotransfer function stored within the ROSETTA database (Schaap et al., 2001). The associated conceptual model comprises a 3 m thick homogenous soil column with an exponentially distributed vertical plant root density distribution contained within the top 1 m of soil. The upper boundary condition comprises a flux associated with the net rainfall rate. The lower boundary condition is represented as a gravity drainage boundary.

An aspect not adequately discussed by Mathias et al. (2015) is the stability of the Euler explicit time-stepping scheme used within the SMAP. Stability is ensured using a scheme very similar to that presented in Appendices B and C of Mathias et al., (2016). Further details about how this is achieved are provided in Appendix A of this article.

Each SMAP simulation was run for a warm-up period of at least 90 days before simulating the period through which observed SMC data is available. An initial value of SMC used to start the warm-up simulation was obtained as follows: First, the SMC that would be expected for a 3 m soil column at hydrostatic conditions with a fictitious water table present at 2 m below the base of the column was determined. The SMAP was then run, with this starting SMC value, using the first three years of net-rainfall and PE data. The final SMC value from this latter simulation was then used as the starting SMC value for the beginning of the 90 day warm-up period.

2.4. Determination of VPR confidence limits

Unconstrained probabilistic estimates of VPR are obtained by performing a Monte Carlo simulation involving uniform random sampling of 10,000 soil textures across the entire soil texture ternary diagram and simulating SMC and VPR for each soil texture realization, for each of the four recharge sites. Cumulative distribution functions for VPR are then obtained to determine values of VPR at each simulation time, which correspond to probabilities of non-exceedance (PNE) of 10% and 90%, hereafter referred to as the P10 and P90, respectively.

2.4.1. Conditioning using the observed soil moisture content (SMC) data

The confidence limits for each VPR are constrained further by conditioning the SMAP to the observed SMC data for each site. This is achieved as follows: The Nash and Sutcliffe (1970) efficiency (NSE) criterion is determined for each realization whereby

$$\mathrm{NSE} = 1 - \frac{\sum_{i=1}^{N}(o_i - m_i)^2}{\sum_{i=1}^{N}(o_i - \overline{o}_i)^2} \tag{1}$$

and N is the number of data points, o_i are the observed SMC data, m_i are the modeled SMC data, and $\overline{o}_i$ is the mean of the observed SMC data.

All the Monte Carlo simulation realizations are ranked in terms of their NSE values. The highest NSE values correspond to those models that gave the most favorable comparison with the observed data. Conditioning is achieved by only retaining the top 10% realizations with the highest values of NSE. Cumulative distribution functions for VPR are then obtained to determine P10 and P90 values of VPR following conditioning.

2.4.2. Conditioning using the UKSO soil texture data

As discussed earlier, soil texture of the surface cover for each of the four sites has been determined at a 1 km scale using the UKSO soil map. UKSO provide a soil texture classification for each location, which is defined in terms of a polygon on a soil texture ternary diagram (recall Fig. 1). As a comparison to conditioning VPR using SMC data, simulated VPR is also conditioned using the UKSO soil texture data. This is achieved by redetermining the P10 and P90 VPR values from the aforementioned full Monte Carlo simulation, whilst only retaining those soil textures contained within the associated UKSO soil texture polygon.

3. Results

Fig. 2 shows the modeling results for Warren Farm. First consider the plots of SMC in Fig. 2a. Note that the plotted lines represent the P10 and P90 results from the unconstrained Monte Carlo simulation, the conditioning on the observed SMC data and the conditioning to the UKSO soil texture classification for that site. For each of the three cases, the P10 and P90 are closely overlain on top of each other suggesting that SMC is completely insensitive to soil texture. Furthermore, the SMAP is able to estimate the observed SMC data to a considerably high-level, regardless of the soil texture assumed.

In contrast, the unconstrained Monte Carlo simulation (the green envelope) presented in Fig. 2b suggests that soil texture has a much more significant effect on VPR, with the difference between the P10 and P90 results being as high as 50% during the peak event of 2004. The difference between the P10 and P90 for VPR clearly narrow following conditioning to the observed SMC data (consider the blue solid lines). However, even with this conditioning, the difference between the P10 and P90 results are as high as 30% during the peak event of 2004. Conditioning the simulations using instead the UKSO soil texture classification leads to a similar level of refinement on VPR. However, conditioning to the UKSO soil texture classification generally leads to a slight overestimation of VPR in 2007 and 2008 as compared to the results obtained by conditioning to SMC data with the exception of the peak VPR events of early 2007 and 2008.

Fig. 3 shows a very similar story for the Highfield Farm site. However, in this case, soil texture conditioning leads to an underestimation of VPR as compared to results obtained by SMC conditioning.

Figs. 4 and 5 show results from Beche Park Wood and Grimsbury Wood, respectively. SMC sensitivity to soil texture is more apparent at these sites (consider the green envelopes in Figs. 4a and 5a). However, SMC data estimates following SMC conditioning and soil texture conditioning at both sites are virtually interchangeable. In contrast, as with Warren Farm and Highfield Farm, there is a much wider variation in VPR estimate.

To gain further insight, Fig. 6 shows the location of all the simulations selected by the SMC conditioning on a soil texture ternary diagram (the blue dots) for each of the four sites considered. The polygons for the associated UKSO soil texture classifications for each of the sites are also shown for comparison (the red solid lines).

From Figs. 6a and b, it is clear that for Warren Farm and Highfield Farm, SMC conditioning identifies soil textures that are completely different to those suggested by UKSO. According to Fig. 1, the SMC conditioning suggests that Warren Farm is more of a "clay to chalky loam" as opposed to a "chalky, silty loam". In the same way, the SMC conditioning suggests that Highfield Farm is more of a "chalky silty loam" as opposed to a "loam to sand".

In contrast, Figs. 6c and d show that some of the soil textures identified by SMC conditioning exist within the allocated UKSO soil texture classification polygons for Beche Park Wood and Grimsbury Wood. It is also notable that the soil log descriptions reported by Sorensen et al. (2014) for these sites are closer to the UKSO descriptions as compared to the soil log descriptions for Warren Farm and Highfield Farm. Recall Sorensen et al. (2014) describes Beche Park Wood as gravely clay and Grimsbury Wood as silty clay. UKSO describe Beche Park Wood as "clay to clayey loam" and Grimsbury Wood as "clay to silt".

Fig. 7 shows contour plots of NSE across the soil texture ternary diagrams for each of the four sites. Note that NSE values closer to one imply better fits to the observed SMC data. Only values of NSE from 0.7 to 0.9 are contoured because 0.9 represents the highest NSE values achieved and less than 0.7 is arguably too poor to consider. The first thing to note is that NSE values greater than 0.7 are achieved at all four sites for all soil textures outside of the UKSO “sand” polygon. Values of NSE within the UKSO “sand” polygon were mostly less than 0.7 for each of the four localities. The next thing to note is that at Warren Farm, NSE was between 0.86 and 0.9 for all soil textures, excluding the UKSO “sand” polygon. NSE values were considerably lower but still exhibit little variability with soil texture at Highfield Farm, Beche Park Wood and Grimsbury Wood.

4. Discussion

The most important observation that can be made from Figs. 2 to 5 is that SMC is virtually insensitive to soil texture. On the other hand, vertical percolation rate exhibits a stronger dependence on soil texture. The above results include a range of different soil type scenarios; consider the UKSO texture classification polygons in Fig. 6. However, all the sites studied are situated in Southern England, and therefore all experience a UK maritime climate. The extent to which climate may be important on the above finding is discussed below.

From an earlier sensitivity analysis of the aforementioned SMAP, Mathias et al. (2015) found that the ratio of AE to PE, averaged over 34 years, ranged from 40% to 94% over the entire soil textural triangle (see their Fig. 5a). However, for sand fraction less than 90% this variation reduced to between just 80% and 94%. The main reason for this is that, in a UK maritime climate, there is generally sufficient rainfall to satisfy evaporative demands. Re-inspection of the governing equations presented by Mathias et al. (2015) reveals that the impact of soil texture on SMC is largely through its control on AE. Because AE is virtually the same regardless of soil texture in this context, very little variation of SMC is observed with changing soil texture.

It is interesting to note that there is marginally more sensitivity of SMC to soil texture at Beche Park Wood and Grimsbury Wood as compared to Warren Farm and Highfield Farm. The main difference between the wooded sites and the farm sites, as far as the SMAP is concerned, is that the wooded sites experience reduced net rainfall due to forest canopy interception losses. Figs. 2c, 3c, 4c and 5c show monthly mean AE (excluding canopy interception loss) and VPR. It is clear that VPR is considerably lower at the wooded sites. Furthermore, whilst AE shows marginal summer variability with soil texture at all four sites, winter variability in AE is only apparent at the wooded sites.

The reduction in available rainfall due to canopy interception makes it harder for plant roots to satisfy evaporative demands. Consequently, the system becomes more dependent on the soil moisture relationship with matric potential and plant stress function (consider Eqs. (22) and (23) in Mathias et al. (2015)). Hence SMC can be seen to me more variable with soil texture at the wooded sites.

The wooded sites can be thought of as a proxy for a slightly more arid climate. It follows that SMC is expected to exhibit a much greater sensitivity to soil texture in semi-arid and arid climates, as compared to UK maritime climates.

With regards to the stronger sensitivity of VPR to soil texture as compared to SMC, VPR is calculated by the SMAP using a non-linear function of SMC (Mathias et al., 2015, Eq. (20)). It follows that any minor variability in SMC will naturally lead to a greater variability in VPR. Conditioning the SMAP to the observed SMC data or the UKSO soil texture classifications leads to a refining of the confidence limits for VPR. However, given the insensitivity of SMC to soil texture, it does not follow that this conditioning leads to increased reliability with regards to VPR.

Similar to the JULES simulations presented by Sorensen et al. (2014), close to zero runoff was estimated by all the models regardless of the soil texture adopted. At Warren Farm the models estimated runoff to occur only on the 27th May 2007 and 20th July 2007 where recorded daily rainfall was 59 and 105 mm, respectively. At the other three sites, runoff was estimated only to occur on the 20th July 2007. Both of these dates have been previously recognized in terms of their high rainfall intensity by Ireson et al. (2011). The reason that the May event is only found to be significant at Warren Farm is due to its relative higher altitude and hence higher rainfall generally. In fact surface runoff was likely to have occurred on many more occasions at Grimsbury Wood and Beche Park Wood due to the nature of the overlying Paleogene deposits (Maurice et al., 2010). However, the modelling approach applied here (and by Sorensen et al. (2014) when using JULES) is not capable of estimating these events due to the use of daily rainfall, which leads to an averaging on rainfall intensities over a 24 hour period (Mathias et al., 2015).

5. Summary and conclusions

In this study, four instrumented recharge monitoring sites previously presented by Sorensen et al. (2014) are revisited to explore the value of observed SMC as a constraint for VPR (a proxy for estimating groundwater recharge rate) estimation. The four sites represent a range of different soil classifications. Although all four sites are from Southern England, two of the sites are located in woodland areas, providing a proxy for a slightly more arid climate.

In their earlier study, Sorensen et al. (2014) concluded that SMC was not a good constraint in this respect. The basis for their argument was that they used four different models to estimate the SMC data and found that, although each model was "generally good" at estimating the SMC data, the different models led to large variations of VPR.

In this article, the observed SMC data has been revisited using a single model structure, the aforementioned SMAP, developed previously by Mathias et al. (2015). Furthermore, rather than just using the SMAP to estimate both SMC and VPR, the model is also calibrated directly to the SMC data to look at how such data can be used to reduce uncertainty associated with VPR estimate.

Monte Carlo simulation using the SMAP suggests that aggregated SMC is virtually insensitive to soil texture. In contrast, uncertainty in soil texture can lead to significant variations in VPR prediction, as high as 50% of P10 values in some cases. Conditioning the SMAP to the observed SMC data or the UKSO soil texture classifications leads to a refining of the confidence limits for VPR. However, given the insensitivity of aggregated SMC to soil texture, it does not follow that this conditioning leads to increased reliability with regards to VPR.

Using a goodness of fit measure, the NSE criterion, it was possible to delineate regions on a soil texture ternary diagram that provide better correspondence between the SMAP and observed SMC at each of the four sites (recall Fig. 6). Interestingly, the delineated regions did not all coincide with the polygons associated with the UK soil observatory (UKSO, 2016) soil texture classifications for the different sites. However, the regions defined by the NSE values represent well defined shapes in all four cases, potentially pointing to an alternative method for defining a "hydrological" soil texture for these sites.

Overall, it is found that the calibrated soil texture values from such an exercise do not always coincide with data from existing field-scale soil texture maps. But more importantly, whilst uncertainty in soil texture can lead to significant uncertainty in groundwater recharge estimation, it is found that aggregated SMC is virtually insensitive to soil texture.

The insensitivity of aggregated SMC to soil texture is largely attributed to the fact that AE is generally not much less than PE in UK maritime climates. However, it is hypothesized that much greater sensitivity of aggregated SMC with soil texture would be observed in arid climates where AE is likely to be much less than PE and more controlled by soil hydraulic properties.

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7. References

Allen, R. G., Pereira, L. S., Raes D., Smith M. (1998), Crop evapotranspiration-guidelines for computing crop water requirements. In FAO Irrigation and drainage, Paper 56, Rome.

Best, M. J., Pryor, M., Clark, D. B., Rooney, G. G., Essery, R., Mnard, C. B. et al. (2011), The Joint UK Land Environment Simulator (JULES), model description–Part 1: Energy and water fluxes, Geoscientific Model Development, 4, 677–699.

Cuthbert, M. O., Acworth, R. I., Andersen, M. S., Larsen, J. R., McCallum, A. M., Rau, G. C., Tellam, J. H. (2016), Understanding and quantifying focused, indirect groundwater recharge from ephemeral streams using water table fluctuations, Water Resour. Res., 52, 827–840.

Feddes, R. A., Kowalik, P., Kolinska–Malinka, K., Zaradny, H. (1976). Simulation of field water uptake by plants using a soil water dependent root extraction function. J. Hydrol., 31, 13–26.

Gash, J. H. C., Lloyd, C. R., Lachaud, G. (1995), Estimating sparse forest rainfall interception with an analytical model, J. Hydrol., 170, 79–86.

Healy, R. W., Cook, P. G. (2002), Using groundwater levels to estimate recharge, Hydrogeol. J., 10, 91–109.

Herbst, M., Rosier P. T. W., McNeil D. D., Harding R. J., Gowing D. J. (2008), Seasonal variability of interception evaporation from the canopy of a mixed deciduous forest, Agric. Forest Meteorol., 148, 1655–1667.

Ireson, A. M., Wheater, H. S., Butler, A. P., Mathias, S. A., Finch, J., Cooper, J. D. (2006), Hydrological processes in the Chalk unsaturated zone–insights from an intensive field monitoring programme, J. Hydrol., 330, 29–43.

Ireson, A. M., Butler, A. P. (2011), Controls on preferential recharge to Chalk aquifers, J. Hydrol., 398, 109–123.

Kerry, R., Rawlins, B. G., Oliver, M. A., Lacinska, A. M. (2009), Problems with determining the particle size distribution of chalk soil and some of their implications, Geoderma, 152, 324–337.

Lott, D. A., Stewart, M. T. (2016), Base flow separation: A comparison of analytical and mass balance methods, J. Hydrol., 535, 525–533.

Mathias, S. A., Butler, A. P. (2006), Linearized Richards' equation approach to pumping test analysis in compressible aquifers, Water Resour. Res., 42, W06408.

Mathias, S. A., Skaggs, T. H., Quinn, S. A., Egan, S. N., Finch, L. E., Oldham, C. D. (2015), A soil moisture accounting-procedure with a Richards' equation-based soil texture-dependent parameterization, Water Resour. Res., 51, 506–523.

Mathias, S. A., McIntyre, N., Oughton, R. H. (2016), A study of non-linearity in rainfall-runoff response using 120 UK catchments, J. Hydrol., 540, 423–436.

Maurice, L., Atkinson, T. C., Williams, A. T., Barker, J. A., Farrant, A. R. (2010), Catchment scale tracer testing from karstic features in a porous limestone, J. Hydrol., 389, 31-41.

Nash, J., & Sutcliffe, J. V. (1970), River flow forecasting through conceptual models part IA discussion of principles, J. Hydrol., 10, 282–290.

Quinn, S. A., Liss, D., Johnson, D., van Wonderen, J. J., and Power T. (2012), Recharge estimation methodologies employed by the Environment Agency of England and Wales for the purposes of regional groundwater resource modelling, Geol. Soc. Spec. Publ., 364, 65–83.

Ragab, R., Finch, J., Harding, R. (1997), Estimation of groundwater recharge to chalk and sandstone aquifers using simple soil models, J. Hydrol., 190, 19–41.

Rutledge, A. T. (2007), Update on the use of the RORA program for recharge estimation, Ground Water, 45, 374–382.

Schaap, M. G., Leij, F. J., van Genuchten, M. T. (2001). Rosetta: A computer program for estimating soil hydraulic parameters with hierarchical pedotransfer functions. J. Hydrol., 251, 163–176.

Sorensen, J. P. R., Finch, J. W., Ireson, A. M., Jackson, C. R. (2014), Comparison of varied complexity models simulating recharge at the field scale, Hydrol. Process., 28, 2091–2102.

UK Soil Observatory (UKSO) (2016), Soil Texture, [ONLINE] Available at: `http://www.ukso.org/pmm/soil_texture.html` [Accessed 17 October 2016].

van Genuchten, M. T. (1980), A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J., 44, 892–898.

von Freyberg, J., Moeck, C., Schirmer, M. (2015), Estimation of groundwater recharge and drought severity with varying model complexity, J. Hydrol., 527, 844–857.

Appendix A. Ensuring stability for the Euler explicit time-stepping scheme

This note provides additional information, not previously reported in Mathias et al. (2015), concerning an Euler explicit time-stepping scheme for the simplified soil moisture accounting procedure (SMAP).

The SMAP of concern involves solving the conservation problem (Mathias et al., 2015)

$$\frac{d\Theta}{dt} = q_r - q_{in} - q_{ro} - q_d - E_a \tag{A.1}$$

where Θ [L] is the aggregated soil moisture content, t [T] is time, q_r [LT^{-1}] is the rainfall rate, q_{in} [LT^{-1}] is the canopy interception rate, q_{ro} [LT^{-1}] is the surface runoff rate, q_d [LT^{-1}] is a drainage rate (which forms an input into a linear reservoir store which outputs the vertical percolation) and E_a [LT^{-1}] is the actual evapotranspiration rate.

Application of an Euler explicit time-stepping scheme leads to

$$\Theta_{n+1} = \Theta_n + \Delta t(q_{r,n} - q_{in,n} - q_{ro,n} - q_{d,n} - E_{a,n}) \tag{A.2}$$

where Δt [T] is the chosen time-step

Following Appendix C of Mathias et al., (2016), it can be shown that stability of the above scheme is ensured providing

$$\frac{\partial}{\partial\Theta}(-q_r + q_{in} + q_{ro} + q_d + E_a) < \frac{1}{\Delta t} \tag{A.3}$$

Note that, according to the equations presented in Mathias et al., (2016), q_r, q_{in} and q_{ro} are independent of Θ. The E_a term is jointly controlled by Θ and the potential evapotranspiration, E_p [LT^{-1}]. It is found that the stability of the above scheme is largely insensitive to E_a, providing E_a is constrained to ensure that $\Theta > \Theta_w$ where Θ_w [L] represents the minimum possible value of Θ associated with plant wilting. In this way, the stability criterion in Eq. (A.3) can be simplified further to

$$\frac{\partial q_d}{\partial\Theta} < \frac{1}{\Delta t} \tag{A.4}$$

Mathias et al. (2015) prescribe that

$$q_d(S_e) = K_s S_e^{\eta}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \tag{A.5}$$

which is the hydraulic conductivity function for unsaturated soils originally proposed by van

Genuchten (1980). K_s [LT^{-1}] is the saturated hydraulic conductivity of the soil, η [-] and m [-] are empirical exponents, and S_e [-] is the effective saturation, estimated by the SMAP using

$$S_e = \frac{\Theta - \Theta_w}{\Theta_{pu}} \tag{A.6}$$

where Θ_{pu} [L] is the soil moisture content capacity available for plant uptake.

Differentiating Eq. (A.5) with respect to Θ leads to

$$\frac{\partial q_d}{\partial \Theta} = \frac{K_s S_e^{\eta-1}}{\Theta_{pu}} \left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 \left[\eta + \frac{2S_e^{1/m}(1 - S_e^{1/m})^{m-1}}{1 - (1 - S_e^{1/m})^m}\right] \tag{A.7}$$

Considering again Eq. (A.4), stability of the scheme is therefore ensured providing $\Theta < \Theta_0$ where

$$\Theta_0 = \Theta_{pu} S_0 + \Theta_w \tag{A.8}$$

and S_0 is found iteratively from the expression

$$\frac{K_s S_0^{\eta-1}}{\Theta_{pu}} \left[1 - \left(1 - S_0^{1/m}\right)^m\right]^2 \left[\eta + \frac{2S_0^{1/m}(1 - S_0^{1/m})^{m-1}}{1 - (1 - S_0^{1/m})^m}\right] = \frac{1}{\Delta t} \tag{A.9}$$

Note that Θ_0 only needs to be found once for each simulation because Θ_0 does not vary with time.

Following Mathias et al., (2016), the above constraint can be imposed by determining the discrete values of q_d from

$$q_{d,n} = \begin{cases} 0, & \Theta_{trial} < 0 \\ q_{d,trial}, & 0 < \Theta_{trial} < \Theta_0 \\ \dfrac{\Theta_n - \Theta_0}{\Delta t} + q_{r,n} - q_{in,n} - q_{ro,n} - E_{a,n}, & \Theta_{trial} > \Theta_0 \end{cases} \tag{A.10}$$

where

$$\Theta_{trial} = \Theta_n + \Delta t(q_{r,n} - q_{in,n} - q_{ro,n} - q_{d,trial} - E_{a,n}) \tag{A.11}$$

with $q_{d,trial}$ being calculated directly from Eq. (A.5) with $S_e = S_{e,n}$.

The reader is referred to Mathias et al. (2015) for all other details concerning the SMAP.

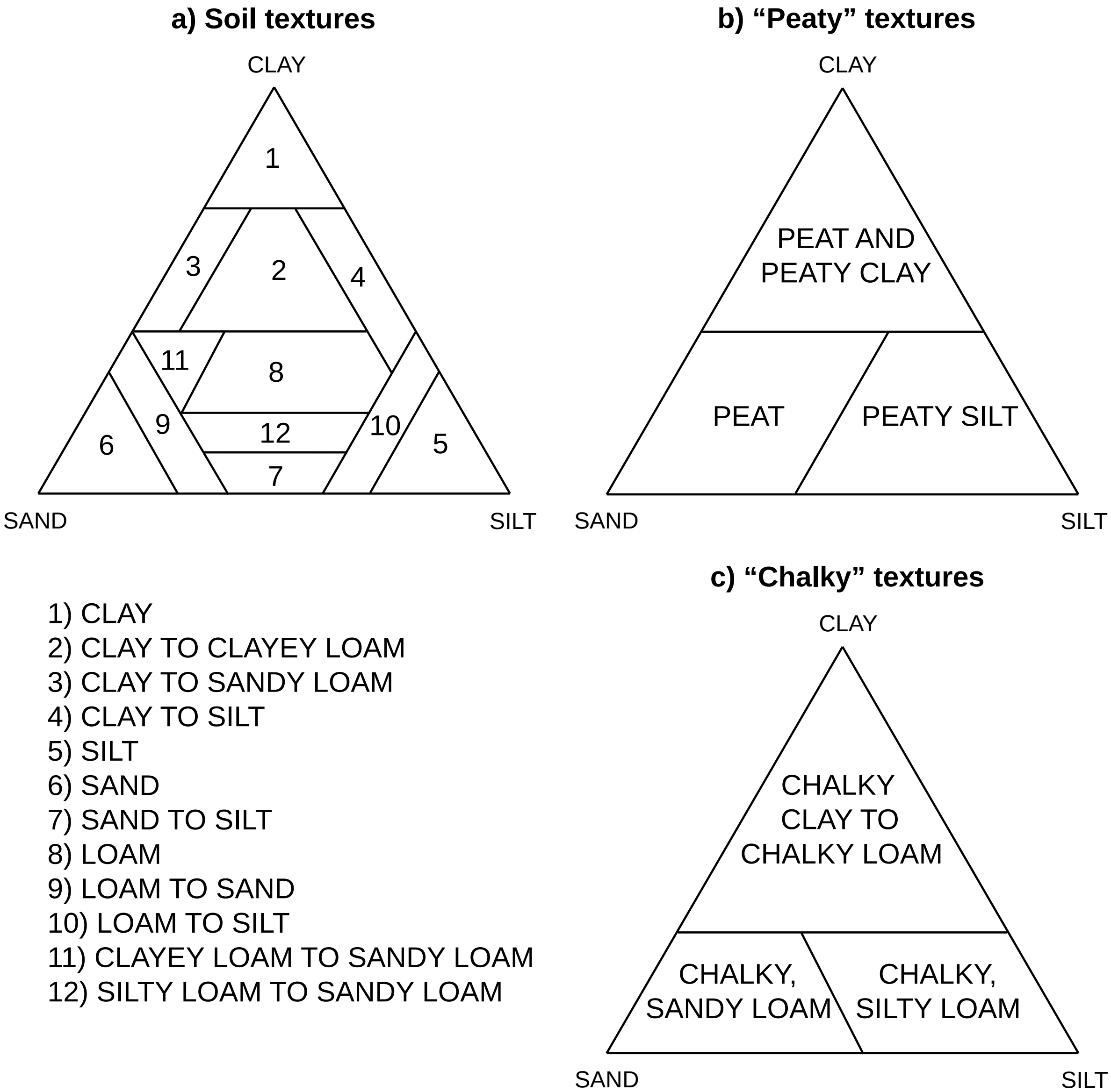

Figure 1: Soil texture ternary diagrams illustrating the various available UKSO soil texture classifications (adapted from UKSO, 2016).

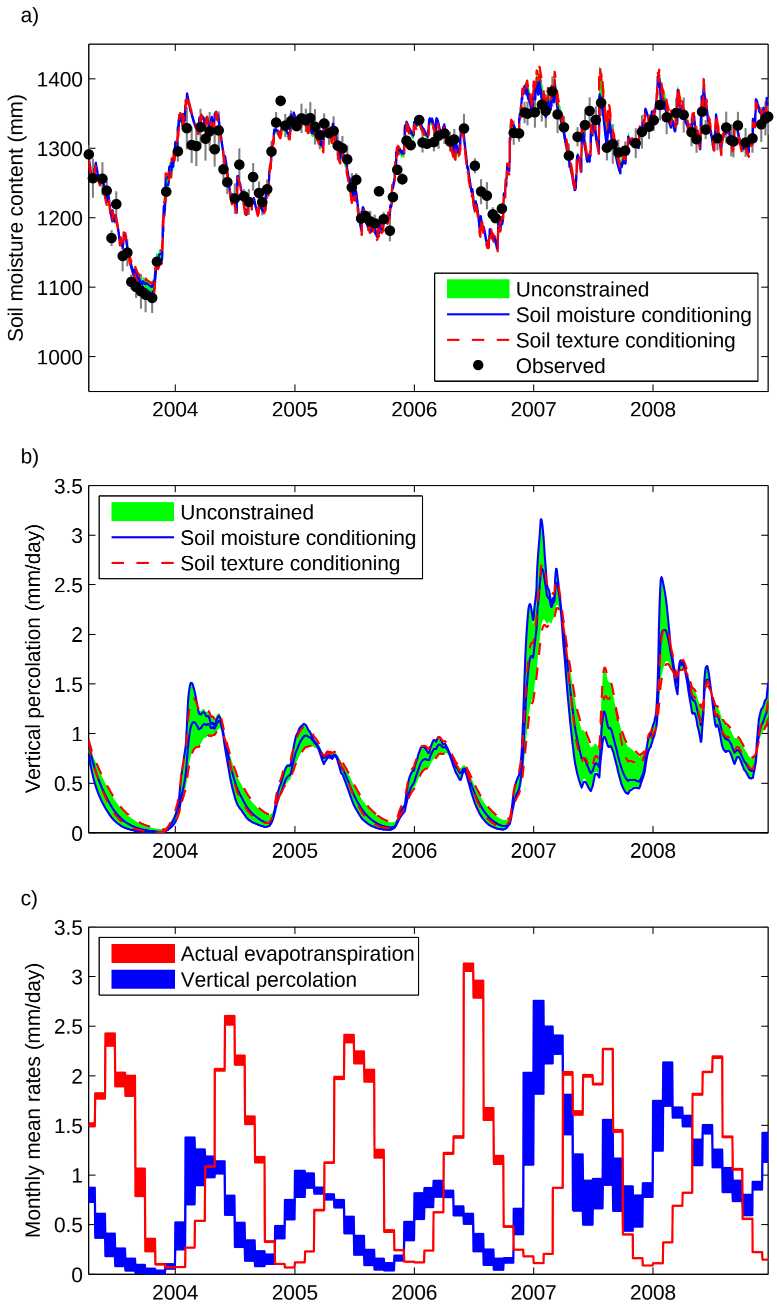

Figure 2: a) and b) Time-series plots of daily soil moisture content and daily vertical percolation rate for Warren Farm. The black dots are the observed soil moisture content data previously presented by Sorensen et al. (2014). The grey bars represent the range in observed soil moisture content, as reported by Sorensen et al. (2014). The green envelope represent the area bounded by the P10 and P90 from the Monte Carlo simulation obtained by uniform sampling across the entire soil texture ternary diagram. The blue lines represent the P10 and P90 of the top 10% of all the simulations in terms of their ability to simulate the observed soil moisture content data. The dashed red lines represent the P10 and P90 of all those simulations that contained soil textures within the UKSO polygon for this site. c) Time-series plots of monthly mean actual evapotranspiration (excluding canopy interception loss) and vertical percolation. The envelopes represent the area bounded by the P10 and P90 from the Monte Carlo simulation obtained by uniform sampling across the entire soil texture ternary diagram.

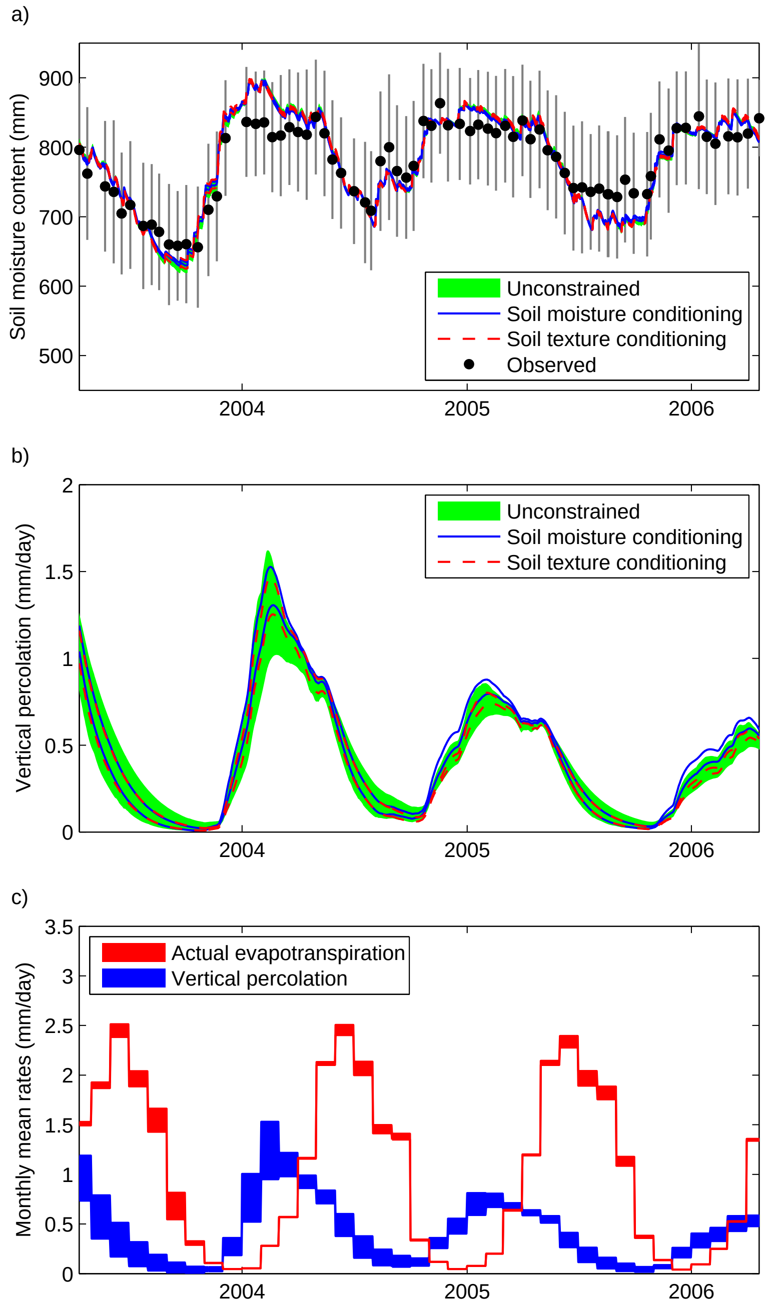

Figure 3: The same as Fig. 2 but for Highfield Farm.

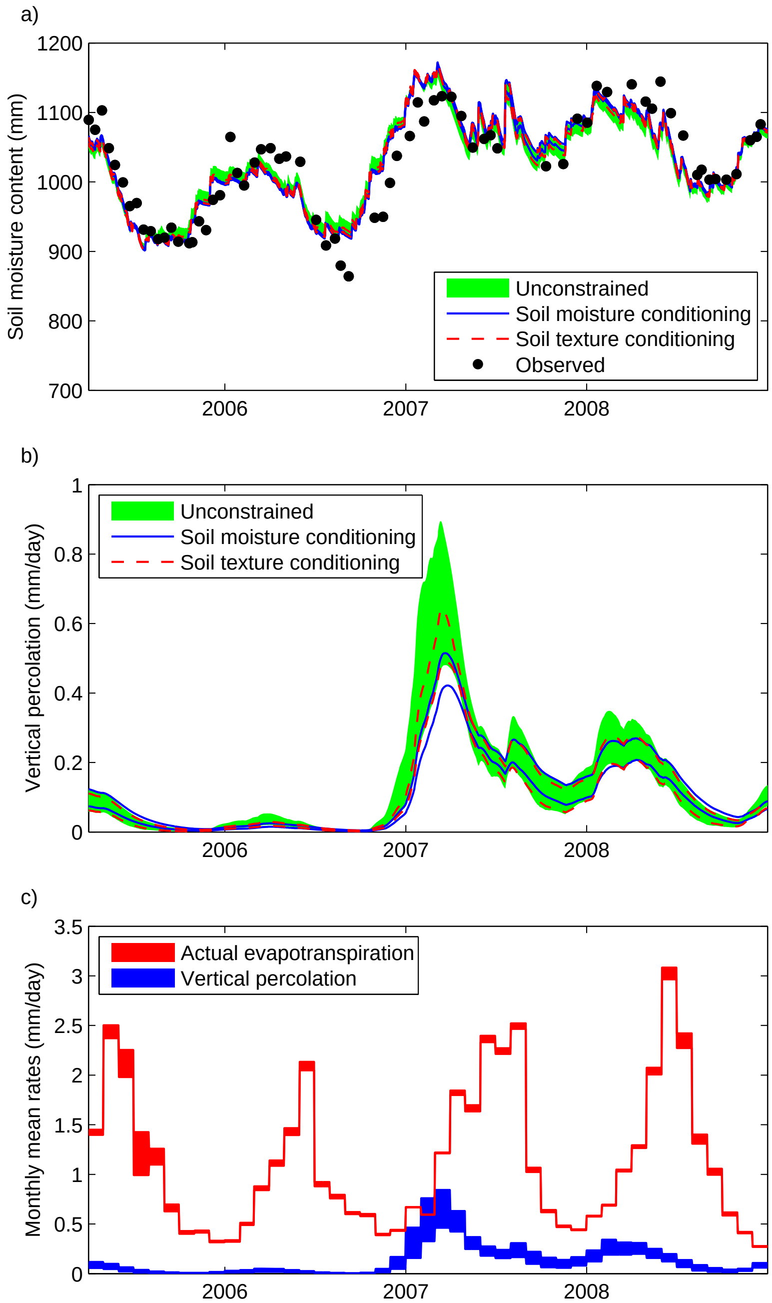

Figure 4: The same as Fig. 2 but for Beche Park Wood.

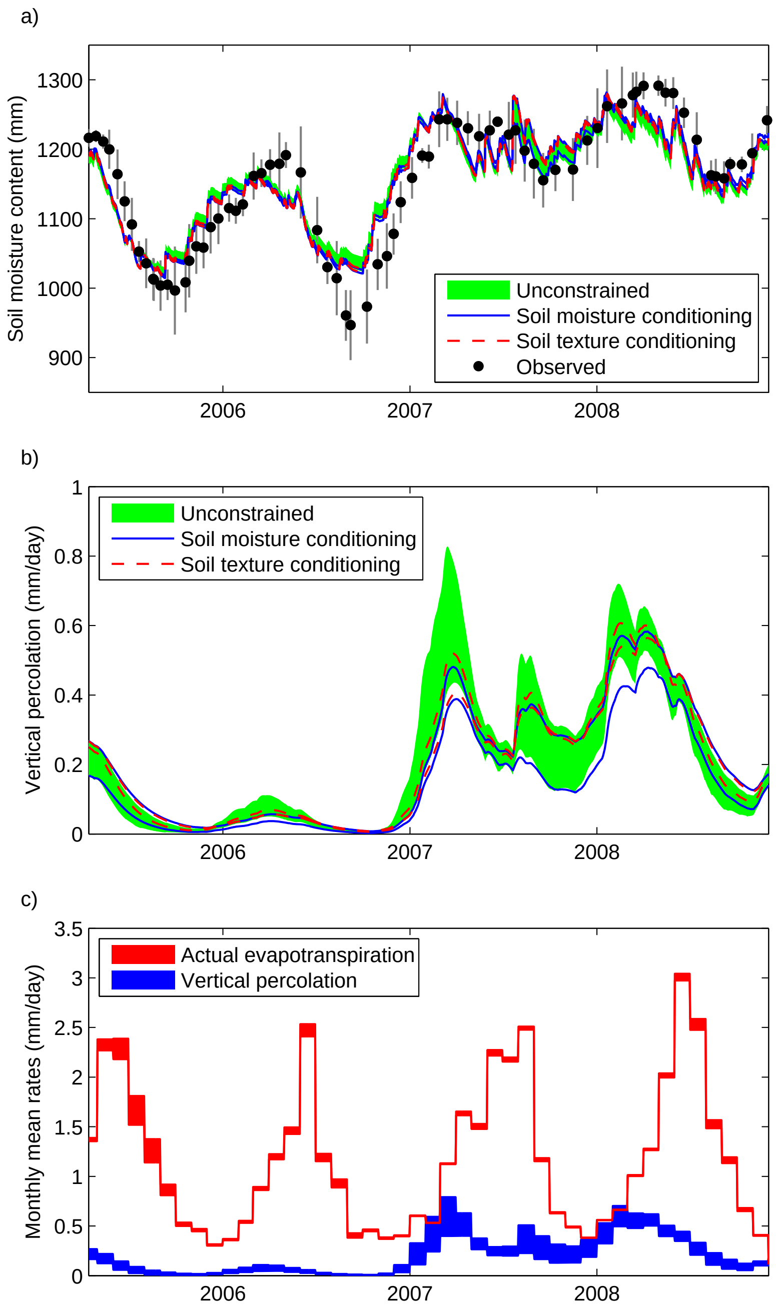

Figure 5: The same as Fig. 2 but for Grimsbury Wood.

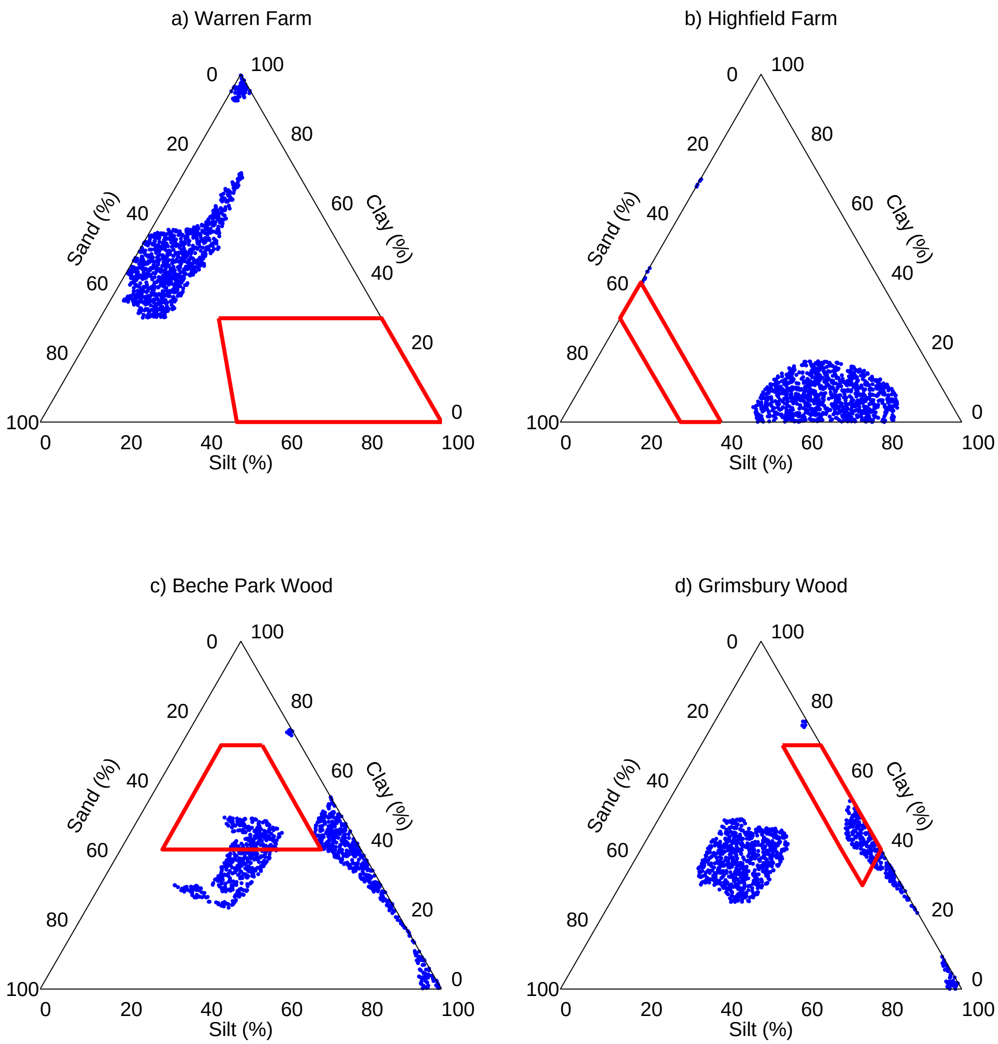

Figure 6: Soil texture ternary diagrams showing blue dots as the locations of the top 10% simulations (in terms of their ability to simulate the observed soil moisture data) for a) Warren Farm, b) Highfield Farm, c) Beche Park Wood and d) Grimsbury Wood. The red polygons denote the region defined by the UKSO soil texture classification associated with each of these sites.

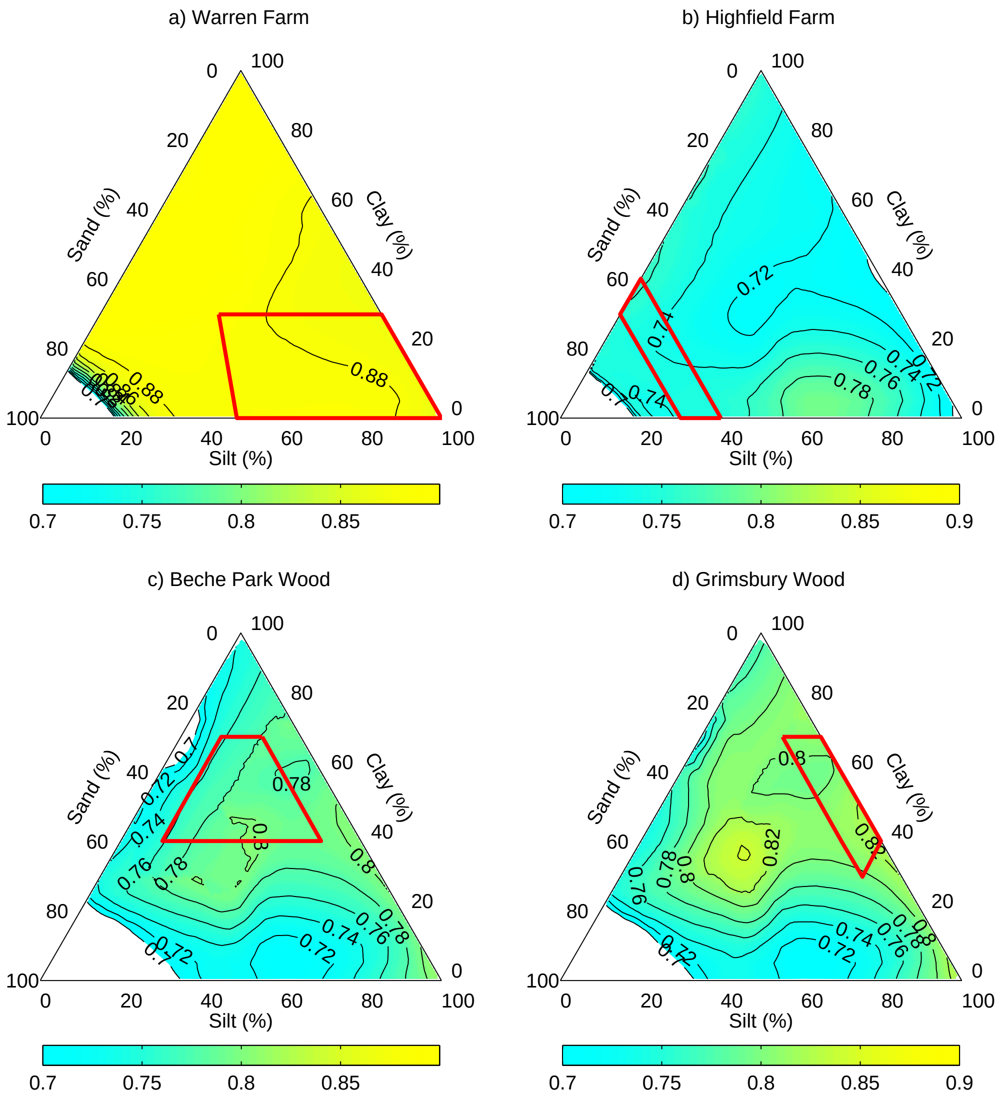

Figure 7: Soil texture ternary diagrams showing Nash and Sutcliffe (1970) efficiency (NSE) contours for a) Warren Farm, b) Highfield Farm, c) Beche Park Wood and d) Grimsbury Wood. The red polygons denote the region defined by the UKSO soil texture classification associated with each of these sites. The color bar values relate to NSE value as given in Eq. (1). Recall that NSE is used here to assess the ability of the models to simulate the observed soil moisture content data.